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Alternative derivations of resistivities at high pressures

A T Oza
Department of Physics, Sardar Patel University,
Vallabh Vidyanagar-388 120, Gujarat, India

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Abstract : Seven organic semiconductors have shown beta density peaks in resistivity against pressure plots. Three polyiodide chain complexes obey $(\rho - \rho_0)/\rho_0 = A + \frac{K(P - A/K)}{1+bP} \exp\left[-c(P - A/K)\right]$ function in d.c. resistivity. Here, alternative derivations of this pressure dependence of resistivity are obtained on the basis of the theory of semiconductors.

Keywords : Organic semiconductors, electrical resistivity, pressure dependence

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1. Introduction

Organic semiconductors like DTN (dithionapthalene), DTN-I_2, anthracene-TNB (TNB = trinitro-benzene) and pyrene-2I_2 reveal beta distributions of resistivity *versus* pressure [1]. Three polyiodine chain complexes follow $\frac{\rho - \rho_0}{\rho_0} = A + K(P - A/K)(1 + bP) \exp\left(-c(P - A/K)\right)$ function which were α-cyclodextrin-KI-I_2, amylose-iodine and (coumarin)$_4$-KI-I_2 [2–5]. AC-resistivities of all the three reveal beta distributions at 1000 Hz. These functions were recently derived from basic theory of semiconductors [2]. Here, five alternative derivations of beta distributions and other functions are given.

2. Theories for beta distributions

(i) Using transfer integral :

The dc resistivities of DTN and DTN-I_2 and ac resistivities of α-cyclodextrin-KI-I_2, amylose-iodine and (coumarin)4-KI-I_2 reveal $\rho/\rho_0 = AP^{*1/2}(1 - P^*)^{1/2}$ where $P^* =$

$(p-a)/b$, a being starting point of the peak and b is base-width of this peak. Thus pressure was converted in the probability of hopping.

The transfer integral for tight-binding approximation is given by $t = IS = Ie^{-r/r_0}$, where S is the overlap integral [6]. Both I and S are modulated by phonons. Here we consider $r = r_i + v_g \mathcal{T}_p$, where $v_g = dr/dt = d\omega/dk$ is the group velocity of lattice vibrations and $\mathcal{T}_p$ is collision time for phonons. The group velocity of acoustic phonons is given by

$$v_g = \frac{d\omega}{dk} = \frac{a}{2}\left(\omega_m^2 - \omega^2\right)^{1/2},$$

where ω_m is the maximum frequency and a is lattice constant [7]. The substitution of v_g and $\mathcal{T}_p = \lambda\nu/\upsilon$, where λ is mean free path, ν is collision frequency and υ is the velocity of free phonons. For a charge density wave, formed by strong electron-phonon coupling $\lambda\nu =$ constant and υ is proportional to $P^{1/2}$ because of $P = 1/3\ mn\upsilon^2$. The conductivity $\sigma = At^2$ then becomes,

$$= AI^2 e^{-2r_i/r_0} \exp\left[-2\frac{a}{2}\frac{1}{r_0}\left(\omega_m^2 - \omega^2\right)^{1/2}\frac{\lambda\nu}{\upsilon}\right],$$

$$\rho = \frac{1}{\sigma} = \frac{1}{AI^2}\exp\left[2r_i/r_0\right]\exp\left[\frac{PK}{r_0}(P_0 - P)^{1/2}\lambda\nu\sqrt{\frac{mn}{3P}}\right].$$

We also substituted $\omega = KP^{1/2}$ since the phonon frequency changes with pressure like this α is linear compression co-efficient. Expansion of exponential leads to

$$\rho = \frac{1}{AI^2}\exp\frac{2r_i}{r_0}\left\{1 + \frac{\alpha K}{r_0}\lambda\nu\sqrt{\frac{mn}{3}}P_0\left(\frac{P}{P_0}\right)^{1/2}\left(1 - P/P_0\right)^{1/2}\right\}.$$

The second term is the required beta density. Here we assume that the ionization potential does not change with pressure. Second type of function, i.e. $\rho/\rho_0 = AP^{*2} \times (1 - P^*)^2$, was found in anthracene-TNB, pyrene-$2I_2$ and in ac resistivities of α-cyclodextrin-KI-I_2, amylose-iodine and (coumarin)$_4$-KI-I_2. For providing this, we follow similar method but the charge carriers couple with lattice polarizability in which ions vibrate like damped and driven oscillator.

$$t^{-2} = I^{-2}\exp\left[\frac{2r_i}{r_0}\right]\exp\left[\frac{2ev_g}{er_0}v_j\right]$$

$$= 1^{-2}\exp\left[\frac{2r_1}{r_0}\right]\exp\left[2E_1 N\left(\frac{i\omega\alpha_e' + \omega\alpha_e''}{er_0}\right)\right],$$

where $\alpha_e'' = \dfrac{e^2\omega\beta/m^{*2}}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\omega\beta/m^*\right)^2}$ and $\beta = \mu\omega^2/6\pi c = B\omega^2$ [8].

Substitutions and $\omega = KP^{1/2}$, $\lambda \sim P$, $v \sim P^{3/2}$, $u \sim P^{1/2}$ and $m^* \sim P^2$ from kinetic theory and degenerate perturbation theory leads to

$$t^{-2} \simeq I^{-2} \exp\left[\frac{2r_i}{r_0}\right] \exp\left[1 + \frac{c}{B^2 r_0 (1/P)\left[(P_0 - P)^2 + 1\right]}\right],$$

$$t^{-2} \simeq I^{-2} \exp\left[\frac{2r_i}{r_0}\right] \exp\left[1 + \frac{cP\left\{1 - (P_0 - P)^2\right\}}{B^2 r_0}\right].$$

Now, the resistivity is given by

$$\rho = \frac{1}{An_0 t^2} = I^{-2} \exp\left[\frac{2r_i}{r_0}\right]\left[1 + \frac{P\left\{1 - (P_0 - P)^2\right\}}{B^2 r_0}\right](E_a^0 - \lambda P)/K_B T$$

because $E_a = E_a^0 - \lambda P$. Now for $r < r_D$ and for one-dimensional hopping $E_a^0 = 1/r_D \rho(E_F)$ is density of states at the Fermi level. This shows that

$$\rho = \frac{1}{AI^2} \exp\left[\frac{2r_i}{r_0}\right]\left[1 + D + K(P_0 - P)^2 E_a^0 P\right.$$

$$\left. + KP^2 (P_0 - P)^2 \lambda + KP^2 \lambda\right],$$

where D and K are constants. Using $r_D = \alpha P$ and $I \sim 1/P$ because I is the difference in Coulomb potentials of two levels, it follows that

$$\rho = \frac{1}{A\beta} \exp\left[\frac{2r_i}{r_0}\right]\left[\frac{(1 + D)}{P^2} + \frac{KP^2 (P_0 - P)^2}{\alpha\rho(E_F)}\right.$$

$$\left. + K\lambda^2 P^2 (P_0 - P)^2 + KP^2 \lambda\right],$$

β is a constant. Third and fourth terms are the leading terms and give rise to beta density peaks. Other trems show monotonic variation without variation without any peak.

Thus in case of acoustic phonons, we assumed λv = constant and for optical phonons of high energy, $\lambda \sim P$ and $v \sim P^{3/2}$ from kinetic theory. Also the ionization potential is unmodified when we consider acoustic phonons and $I \sim 1/P$ when optical phonons are considered because optical phonons are related with ionization.

(ii) Using Slater orbitals :

Slater orbitals are described by radial part of the wave function, *i.e.*

$$R(r) = Nr^{n-1} \exp\left[-\mu' r/a_0\right],$$

where μ' is a constant, N is normalization constant, n is quantum number and a_0 is Bohr radius [9]. Using $r = r_i + \left(\frac{dr}{dt}\right)T_p$ gives

$$R(r) = Nr^{n-1}\exp\left[-\mu' r/a_0\right]\exp\left[\frac{\mu'}{a_0}\frac{a}{2}(\omega_m^2 - \omega^2)^{1/2}\left(\frac{\lambda v}{v}\right)_t\right]$$

Now, the resistivity is given by

$$\rho = \frac{1}{Q\mu} - \frac{1}{e|R|^2\mu}$$

$$= \frac{m^*}{e^2\mu}\left(\frac{v}{\lambda v}\right)_e \frac{1}{N^2 r^{2(n-1)}}\exp\left[2\mu' r_i/a_0\right]\left[1 + \frac{\mu'}{a_0}p^{1/2}(p_0 - p)^{1/2}\right],$$

λv = constant for phonons and $v \sim p^{1/2}$ is used and exponential term is expanded to first order. Now,

$$r^{2(n-1)} = r_0^{2(n-1)}[1 + \alpha p]^{2(n-1)} \simeq A[1 + 2\alpha(n-1)p],$$

$v \sim p^{1/2}$, $v \sim p^{3/2}$ and $\lambda = h/p$ for charge density wave, where λ is constant limited by the wavelength of charge density wave. These considerations lead to

$$\rho = A + Bp^{1/2}(p_0 - p)^{1/2}$$

which is nothing but beta density.

For the other type of beta density, electronic motions couple with lattice polarizability,

$$\rho = \frac{1}{e}\frac{m^*}{e}\left(\frac{v}{\lambda v}\right)_p \frac{1}{N^2 r^{2(n-1)}}\exp\left[\frac{2\mu'}{a_0}\frac{E_1 N}{e}(i\omega\alpha_c' + \omega\alpha_c'')(\lambda v/v)_p\right].$$

The substitutions for pressure dependence leads to

$$\rho = c\left[1 + \frac{2\mu' N\alpha p^3}{a_0 e[(p_0 - p)^2/p + 1]}\right],$$

$$\rho \simeq c\left[1 + \frac{2\mu' N\alpha p^3}{a_0 e}\{1 - (p_0 - p)^2/p\}\right].$$

The second term has p^3 dependence but third term is beta density, *i.e.* $p^2(p_0 - p)^2$. In getting p^3, $\exp(-\beta p/KT)$ is expanded up to first order using $E_a = E_a^0 - \beta p.\lambda_{el}$ is assumed to be constant as it is limited by wavelength of charge density wave.

(iii) Form density of states :

Here, $D(E) \sim |E - E_c|^{-1/2}$ for square-well potential and $D(E) \sim \ln|E - E_c|$ for sine-wave potential are used as discussed elsewhere for deriving beta densities [10]. Pressure creates a fluctuation in the energy because of non-equilibrium conditions.

$$E = E_0 + \frac{dE}{dn}\Delta n = E_0 + \Delta n\beta\left|E - E_c\right|^{1/2}$$

Now, $$\rho = \rho_0 e^{\left(E_a + \Delta n\beta\left|E - E_c\right|^{1/2}\right)/K_B T} = \frac{m^* v}{n_0 e^2 \lambda v} \exp\left(E_a + \Delta n\beta\left|E - E_c\right|^{1/2}\right)/K_B T$$

$$m^* \sim p^2, E_a = E_a^0 - \beta p,$$

v = constant for a CDW, $\lambda \sim p$ and $v \sim p^{1/2}$ gives

$$\rho \simeq Ap^{1/2}(1-p)^{1/2},$$

where A is a constant. This is the beta density of the first type. For the other type,

$$\rho = \frac{m^* v}{n_0 e^2 \lambda v} \exp\left(E_a^0 - \beta p\right) \quad \beta \ln\left|E - E_c\right|^{\Delta n}\Big/ K_B T.$$

The expansion of $\exp\left(1/\ln\left|E - E_c\right|\right)$ gives a term proportional to $\left|E - E_c\right|^2$ using Laurent expansion and other $|E|^2$ factor is obtained by usual substitutions. Now energy is work done by pressure, which leads to beta density of the type

$$\rho \simeq A + \beta p^{*2}(1 - P^*)^2,$$

where $$p^* = E/E_c.$$

(iv) From physical kinetics :

Here, we consider that the displacements of electrons and phonons in charge density waves are limited by de Broglie wavelength.

$$J = \sigma E = nev = nei\omega(x_1 + x_2),$$

$x_1 = h/p_e$ and $x_2 = h/p_p$. Thus

$$\rho = \frac{p_e p_p}{i\omega n_0 eh(p_e + p_p)} \exp\left[E_a - \lambda p\right]/K_B T,$$

$p_e + p_p$ is the total momentum CDW and

$$p_e = \sqrt{2m^*\left[E_g - (E - V)\right]} \text{ and } p_p = \sqrt{2m^*(E - V)},$$

because p_e is the momentum of electrons in conduction band. Expanding the exponential up to first order and substitutions $m^* \sim p^2$, $\omega \sim p^{1/2}$, $(p_e + p_p) \sim p^{5/2}$ because $m^* \sim p^2$ and $v \sim p^{1/2}$ leads to

$$\rho \simeq A + B^{*1/2}(1 - p^*)^{1/2},$$

where $p^* = (E - V)/E_g$. This is the beta density.

For other type of beta density involving squares of energy, needs relativistic kinetics.

$$\rho \simeq \overline{in_0 \omega eh(p_e + p_p)} \exp\left[\frac{1}{2}\gamma m v^2/kT + E_g/kT\right]$$

$$\sim \frac{E_R^2 - m^{*2}c^4}{ip^{1/2}n_0 c^2 eh 2p^{5/2}}(1 + \beta p/2c^2)\exp\left[E_a - (E-V)\right]/kT$$

$$\sim \frac{E_R^2 - \alpha c^4 p^4(1 + \beta P/2c^2)}{ip^{1/2}2n_0 c^2 eh 2p^{5/2}}\left[1 - \frac{E_a - (E-V)}{kT} + \frac{1}{2!}\frac{[E_a - (E-V)]^2}{(kT)^2}\right],$$

where $v^2 = \beta p$ is substituted and the exponential is expanded.

The leading term leads to

$$\rho \sim \frac{(1-p^*)^2 p^{*2} E_a^4}{in_0 eh(kT)^2},$$

where $p^* = (E-V)/E_a$.

This explains why the pressure breadth (Full width at half maximum) linearly scales with activation energies as found for six complexes [2].

Other way to bring squares of energy which can be replaced by pressure as work done is to consider first or second-order perturbation theory. Here,

$$W = E_m + \frac{|\langle m|H'|m\rangle|^2}{E_m - E_n}$$

and

$$\psi^*\psi = 1 + \frac{|\langle m|H'|m\rangle|^2}{(E_m - E_k)^2}$$

as considered elsewhere [11]. Now

$$\rho = \frac{m^* v}{n_0 e^2 \lambda v}\exp\left[-W/kT\right]$$

$$\simeq \frac{m^* v}{n_0 e^2 \lambda v}\left[1 - E_m + |\langle m|H'|m\rangle| - \frac{|\langle m|H'|m\rangle|^2}{\Delta E}\right.$$

$$\left. + E_m^2 + 2E_m\langle m|H'|m\rangle + |\langle m|H'|m\rangle|^2\right]$$

by expanding the exponential up to second power. Other way is to use $\psi\psi^*$ in

$$\rho = \frac{1}{ne^2|\psi|^2\mu}$$

$$\simeq \frac{1}{n_0 e\mu}\left[1 - \frac{|\langle k|H'|m\rangle|^2}{(\Delta E)^2}\right]\exp\left[-W/kT\right].$$

Again $\exp[-W/kT]$ can be expanded. Later $|\langle k|H'|m\rangle|^2$ gives $[E_g - (E-V)]^2$ term and $|E-V|^2$ is obtained by other substitutions and expansion of $\exp[-W/kT]$. The elastic energy is proportional to pressure as work done by pressure.

(v) Using absorption coefficients :

For direct transition, the absorption coefficient is given by

$$K = 0.115\left(\frac{E_g e^2 m^{*1/2}}{h\nu c_0}\right)(h\nu - E_g)^{1/2}$$

as taken from elsewhere [12]. $h\nu$ is energy of light to be replaced by elastic energy supplied by pressure. $E_g = E_g^0 - \alpha p$. Now $\sigma = Kn_1 c/4\pi$, $n_1 = \sqrt{\varepsilon\mu}$, $\varepsilon = 1 + \lambda^2/k^2$, where $\lambda^2 = 6\pi n_0 e^2/\varepsilon_F$ (λ is screening constant) [13] gives $\varepsilon \sim 1/p$ and $n_1 \sim 1/\sqrt{p}$. This leads to

$$\sigma = Kn_1 c/4\pi$$

$$= 0.115\frac{\beta(E_g^0 - \alpha p)e^2 p}{pc_0 \hbar^2}(E - E_g)^{1/2}\frac{n_1 c}{4\pi}.$$

AC conductivity increases, when dc conductivity decreases. The second term gives beta density of the type $\sigma = A + Bp^{*1/2}(1-p^*)^{1/2}$ where $p^* = E/E_g$.

For an indirect transition [12]

$$k = \frac{e^2(m_c^* m_v^*)^{3/2} B^2 \langle \varepsilon_a - \varepsilon_f \rangle_{av}}{2\pi n c_0 \hbar^2 \omega^2 \langle \varepsilon_a - \varepsilon_f \rangle_{av}^2} \sum (\omega - E_g \pm k\theta)^2 .$$

where $B = (\hbar^2/m^*)\int u_s \frac{\partial}{\partial j} u_j dq,$

$\langle \varepsilon_i - \varepsilon_f \rangle_{av}$ and $\langle \varepsilon_a - \varepsilon_f \rangle_{av}^2$ are pressure independent. $m^* \sim p^2$, $\hbar\omega$ is replaced by elastic energy E, and $\beta^2 \sim 1/m^{*2} \sim 1/p^4$ leads to

$$K = A\sum (E - E_g \pm k\theta)^2 \quad N_s^2 M_s^2 \text{ or } (N_s^2 + 1)M_s^2.$$

Now, $M_s N_s^2$ or $M_s^2(N_s + 1)$ is $|\langle f|h_1|a\rangle|^2$ *i.e.* perturbation potential is replaced by constant × (pressure)^2 as work done providing the elastic energy. Thus,

$$K = A\beta^2(1 - p^*)p^{*2},$$

where $E = \beta p$ and $p^* = (E \pm k\theta)/E_g$.

This is the required function. Now for semiconductor, resistivity rather than conductivity is proportional to absorption coefficient. This can be understood by dielectric loss in complex Poyinting Theorem [14]. Thus if K is beta density, the resistivity will have same form.

3. Theory for other pressure dependences

In the dc resistivity of α-cyclodextrin-KI-I_2, amylose-iodine and (coumarin)$_4$-KI-I_2, it was found that

$$\frac{\rho-\rho_0}{\rho_0} = A + \frac{k(p - A/k)}{1 + bp} e^{-c(p-A/k)},$$

where k, b and A are constants [2]. This relation can be derived from theory of lattice vibrations, *i.e.* phonons, as found elsewhere [15]. For acoustic and optical phonon modes, the general equation is [15]

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1 - \cos ka) = 0.$$

A direct differentiation leads to

$$v_g = \frac{d\omega}{dk} = \frac{C^2 a}{2\omega} \frac{\sin ka}{\left[4M_1 M_2 \omega^2 - C(M_1 + M_2)\right]},$$

C is elastic constant, α lattice constant and M_1 and M_2 are masses of vibrating atoms. sin ka is treated as independent of pressure.

$$\rho = \frac{m^* v}{n_0 e^2 \lambda v} \exp\left(\frac{E_a^0}{kT} - \frac{\lambda' p}{kT}\right)$$

$$\sim \frac{p^2}{n_0 e^2 \lambda p^{3/2}} \frac{p^{1/2} \exp\left(E_a^0/kT - \lambda' p/kT\right)}{\left[4M_1 M_2 p - C(M_1 + M_2)\right]} \left(\frac{c^2 a}{2\omega}\right)$$

$$\sim \frac{kp}{1+bp} \exp\left[-cp\right],$$

where $b = -4M_1 M_2 \beta / C(M_1 + M_2)$ and $c = \lambda'/kT$.

Here, we assume that the mean free path λ is limited by wavelength of a CDW and therefore, it is independent of pressure. The elastic constant C weakly depends on pressure.

The other types of pressure dependence was found in N_i $(H\ dmg)_2$ and N_i $(H\ dpg)_2$ and *dmg* = dimethylglyoxime and *dpg* = diphenylglyoxime. Here, work Gaussians were found in high pressure [16]. *i.e.*

$$\rho = \rho_0 \exp\left[-(p - p_0)^2 / 2W\right],$$

where W is width of Gaussian. Now $\rho = \rho_0 e^{E_a/kT}$. A direct differentiation gives,

$$\frac{d\rho}{dp} = \frac{\partial \rho_0}{\partial p} \exp\left[E_a/kT\right] + \rho_0 \left(\frac{1}{kT}\right)\left(\frac{\partial E_a}{\partial p}\right) \exp\left[E_a/kT\right].$$

This does not give dE_a/dp over the exponential, so we should write

$$E_a = E_{ai} + \left(\frac{\partial E_a}{\partial p}\right)\Delta p,$$

as a function in activation energy brought about by non-equilibrium process induced by applied pressure.

Also $$E_a = E_{ai} + \left(\frac{\partial E_a}{\partial p}\right)_0 (\Delta p) + \frac{1}{2!}\left(\frac{\partial^2 E_a}{\partial p^2}\right)_0 (\Delta p)^2,$$

where $\Delta p = p - p_0$. The third term in $(\Delta p)^2$ when goes over exponential, gives a Gaussian distribution where the width is determined by $(\partial^2 E_a/\partial p^2)_0$. Now in the case of anthracene-TNB a normal distribution is found at low pressure which is integration of a Gaussian. Here we should consider fluctuation.

$$\frac{\partial E_a}{\partial p} = \left(\frac{\partial E_a}{\partial p}\right)_0 + \frac{1}{2!}\left(\frac{\partial^2 E_a}{\partial p^2}\right)_0 2(\Delta p).$$

This can be substituted in the non equilibrium equation, *i.e.*

$$E_a = E_{ai} + \left(\frac{\partial E_a}{\partial p}\right)\Delta p = E_{ai} + \left(\frac{\partial^2 E_a}{\partial p^2}\right)(\Delta p)^2.$$

This Gaussian distribution can be explicitly obtained using transfer integral and oscillator model for polarisability as follows.

$$\rho = \frac{1}{At^2} = \frac{1}{AI^2 \exp[2/a_0](dr/dt)\tau_p \exp[2r_1/a_0]}$$

$$= C\exp\left(\frac{2ev}{a_0 e}\tau_p\right) = C\exp\left[\frac{E_1 N(i\omega\alpha_e' + \omega\alpha_e'')\tau_p}{a_0 e}\right].$$

Substituting α_e'' from oscillator model as done earlier one gets

$$\rho = C\exp\left(\frac{2E_1 N}{a_0 e}\left[\frac{(\omega^2 e^2 \beta/m^{*2})\tau_p}{(\omega\beta/m^*)^2\left\{(\omega_0^2 - \omega^2)^2/(\omega\beta/m^*)^2 + 1\right\}}\right]\right).$$

Substituting $\beta = A\omega^2$, $m^* \sim p^2$ and, one gets

$$\rho = C\exp\left(\frac{2E_1 N}{a_0 e}\left[\frac{p^{1/2}Ae^2\, p^{3/2}/p^4}{A^2 p^3/p^4}\left\{1 - \frac{k(p_0 - p)^2}{A^2 p^3/p^4}\right\}\tau_p\right]\right).$$

The first term goes as exp $[B/p]$ where B is a constant. This term has no peak. The second term is exactly a Gaussian with $(p_0 - p)^2$ over the exponential. In this way, the Gaussian curves found in N_i (*H dpg*) and N_i (*H dmg*)$_2$ elsewhere [16] can be proved mathematically. The Gaussian can be proved using Slater orbitals and other methods involving an exponential in similar manner.

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